

# Comment on “Absence of spin liquid in non-frustrated correlated systems”

Ansgar Liebsch

*Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany*

In a recent Letter, Hassan and Sénéchal [1] discussed the existence of a spin-liquid phase of the half-filled Hubbard model on the honeycomb lattice. Using schemes, such as the variational cluster approximation (VCA) and the cluster dynamical mean field theory (CDMFT) in combination with exact diagonalization (ED), they argued that a single bath orbital per site of the six-atom unit cell is insufficient and leads to the erroneous conclusion that the system is gapped for all nonzero values of the onsite Coulomb interaction  $U$ . In contrast, we point out here that, in the case of the honeycomb lattice, six bath levels per six-site unit cell are perfectly adequate for the description of short-range correlations. Instead, we demonstrate that it is the violation of long-range translation symmetry inherent in CDMFT-like schemes which opens a gap at Dirac points. The gap found at small  $U$  therefore does not correspond to a Mott gap. As a result, present CDMFT schemes are not suitable for the identification of a spin-liquid phase on the honeycomb lattice.

As shown in Ref. [2], the cluster self-energy obtained within ED CDMFT [3] using six bath levels is in nearly quantitative agreement with results derived within continuous-time quantum Monte Carlo (QMC) CDMFT [4]. As the bath in QMC is infinite, the self-energy is not subject to finite-size effects. The reason for the good agreement is that, because of the semi-metallic nature of the honeycomb lattice, the projection of the infinite-lattice bath Green's function onto a finite-cluster Anderson Green's function is not plagued by the low-energy-low-temperature disparities that arise in the case of correlated metals and the square-lattice Hubbard model. Moreover, because of the hexagonal symmetry, this projection can be performed in the diagonal molecular-orbital basis with non-symmetrical density of states components [3]. The main issue in Ref. [1] concerning the symmetry of bath levels then does not arise and the two independent bath Green's function components are fitted accurately using a total of six parameters (see Fig. 24 of Ref. [2]), while in the site basis only one fit parameter is available.

Within CDMFT, the self-energy at Dirac points  $K$  exhibits the low-energy behavior [3]:  $\Sigma(K, i\omega_n) \approx ai\omega_n + b^2/[i\omega_n(1-a)]$ , where  $a$  is the initial slope of  $\text{Im}[\Sigma_{11}(i\omega_n) - \Sigma_{13}(i\omega_n)]$  and  $b$  the low-energy limit of  $\text{Re}[\Sigma_{12}(i\omega_n) - \Sigma_{14}(i\omega_n)]$ . Here,  $\Sigma_{ij}$  is the self-energy in the site basis and  $\omega_n$  are Matsubara frequencies. The excitation gap at temperatures  $T \rightarrow 0$  is given by  $\Delta \approx 2|b|/\sqrt{1-a}$  (see also Ref. [5]). Using the site notation:  $\mathbf{a}_1 = (0, 0)$ ,  $\mathbf{a}_2 = (0, 1)$ ,  $\mathbf{a}_3 = (\sqrt{3}/2, 3/2)$ ,  $\mathbf{a}_4 = (\sqrt{3}, 1)$ ,  $\mathbf{a}_5 = (\sqrt{3}, 0)$ , and  $\mathbf{a}_6 = (\sqrt{3}/2, -1/2)$ , the elements  $\Sigma_{12}$  and  $\Sigma_{14}$  within this cell are indepen-

dent, so that  $\Delta \neq 0$ . However, site 1 is also connected to site 4 at  $(-\sqrt{3}/2, -1/2)$  in the neighboring cell, requiring  $\Sigma_{12} = \Sigma_{14}$  which is not obeyed in CDMFT. Therefore, this violation of translation symmetry is responsible for the insulating contribution  $\sim 1/i\omega_n$  to the self-energy at  $K$ . Clearly, this term is not caused by the finite size nor the symmetry properties of the bath employed in ED. In fact, in view of the good agreement with ED, the self-energy in QMC CDMFT [4] exhibits the same insulating contribution, so that the density of states should also reveal a gap at small  $U$  and low  $T$ .

To restore translation symmetry, we have performed ED calculations within the dynamical cluster approximation (DCA). This approach ensures  $\Sigma_{12} = \Sigma_{14}$ , giving semi-metallic rather than insulating behavior at small  $U$  [6]. The condition  $\Sigma_{12} = \Sigma_{14}$ , however, cannot be generally correct for correlations within the unit cell. The critical Coulomb interaction  $U_c \approx 6$  found in DCA should therefore be used with caution.

For interactions in the range  $U \approx 4 \dots 5$ , ED and QMC CDMFT [3,4] yield excitation gaps which agree remarkably well with the charge gap derived in large-scale QMC calculations [7]. Evidently, this gap corresponds to a Mott gap induced by short-range correlations and is only weakly affected by the lack of long-range translation symmetry. On the other hand, the key question as to how this gap closes, i.e., how the semi-metallic phase with weakly distorted Dirac cones is recovered at small  $U$ , cannot be studied adequately within CDMFT. The gap obtained at small  $U$  is an artifact caused by the violation of long-range lattice symmetry and does not represent a true Mott gap. As a result, the identification of a spin-liquid phase on the honeycomb lattice is presently not feasible within CDMFT-like methods.

In conclusion, the origin of the narrow excitation gap at small  $U$  found in ED CDMFT for the honeycomb lattice is not the finite bath as stated in Ref. [1] but the lack of translation symmetry. This problem is also shared by QMC CDMFT and can be avoided, for instance, within ED/QMC DCA.

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